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MEMORANDUM REPORT NO. 2763

VIGOROUS IGNITION DYNAMICS REVISITED

Carl W. Nelson

June 1977

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USA ARMAMENT RESEARCH AND DEVELOPMENT COMMAND
USA BALLISTIC RESEARCH LABORATORY
ABERDEEN PROVING GROUND, MARYLAND

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The NOVA code developed by Gough is applied to the two phase flow problem of a detonating igniter for a packed bed of solid propellant grains. Previous computations and theory of Krier are compared with computations and theory by Gough. Pressure propagation rate predictions by NOVA are twice those of Krier, but still lower than experimental rates. Gas temperature profiles are markedly different.

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LIST OF SYMBOLS

A	cross sectional area
e	internal energy
E	total energy
e_{chem}	heat release in combustion
$\dot{m}_b$	mass burning rate
p	static pressure
R	stress tensor
u	gas velocity
u_p	particle velocity
u_m	mixture velocity
q_{gp}	heat transfer from gas to particles
q	heat loss from system
t	time
x	axial distance
ϕ	porosity
$\mathcal{D}$	interphase drag
ρ	gas density
ρ_p	solid density
ψ	external mass input rate

INTRODUCTION

Several researchers have produced models to predict the flame spreading and pressurization of mobile bed of solid propellant. A heated debate over the correctness of the governing equations has divided into two sides - The University of Illinois[1] model against others (Kuo[2], Gough[3], and Fisher[4]). In addition to two other applications[5,6], Krier and associates[7] have applied their model to a BRL laboratory experiment[8] which detonated a tetryl pellet at one end of a circular cylinder filled with M30 propellant.

It is the purpose of this report to criticize Krier's computational results and to present the different results predicted by Gough's model. Direct linkage of differences in theory with differences in results will not be made here because it is still too complicated. This report will provide one piece of limited information on the two-phase flow modeling debate.

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[1] *W. VanTassell and H. Krier, "Combustion and Flame Spreading Phenomena in Gas-Permeable Explosive Materials", Intl J Heat Mass Transfer, 18 (12), p1377-1386, 1975.*

[2] *K. K. Kuo, J. H. Koo, T. R. Davis, and G. R. Coates, "Transient Combustion in Mobile Gas Permeable Propellants", Acta Astronautica 3, p573-591, 1976.*

[3] *P. S. Gough, "Numerical Analysis of a Two Phase Flow with Explicit Internal Boundaries", Paul Gough Associates PGA-TR-76-2, September 1976.*

[4] *E. B. Fisher, K. W. Graves, and A. P. Trippe, "Application of a Flame Spread Model to Design Problems in the 155mm Propelling Charge", 12th JANNAF Combustion Meeting, Newport, RI, CPIA Publication 273, December 1975.*

[5] *M. W. Beckstead, N. L. Peterson, D. T. Pilcher, B. D. Hopkins, and H. Krier, "Convective Combustion Modeling Applied to Deflagration-to-Detonation Transition", 12th JANNAF Combustion Meeting, Newport, RI, CPIA Publication 273, December 1975.*

[6] *H. Krier, S. Rajan, and W. F. VanTassell, "Flame Spreading and Combustion in Packed Beds of Propellant Grains", AIAA J 14(3), March 1976.*

[7] *H. Krier and S. S. Gokhale, "Predictions of Vigorous Ignition Dynamics for a Packed Bed of Solid Propellant Grains", Intl J Heat Mass Transfer, 19 p915-923, 1976.*

[8] *J. D. Knapton, I. C. Stobie, and R. H. Comer, "Vigorous Ignition of M30 Propellant", BRL Memorandum Report No. 2662, August 1976, AD #B013322L.*

It has recently come to this author's attention that a similar debate is raging in the two phase industrial heat transfer community. Although the intensity of the physical processes is much less there, debate on formulation of the conservation equations is perhaps more intense than in the gun community. For example see Reference 9.

EXPERIMENTAL

Theoretical Differences

Conservation equations for the Illinois model are derived from the principles of continuum mechanics; Gough's equations are derived from a formal averaging procedure for two separate phases. Term by term comparison of the equations has been reported by Kuo[10]. Although the equations for mass conservation are the same for both, the equations for momentum and energy conservation are different.

Controversial "diffusion" terms in Krier's momentum and energy equations arise from an assumption of an inviscid, Newtonian mixture. Having assumed inviscid, Newtonian components, Gough derives no such terms in his equations. Although Beckstead et al[5] showed an indifference to the presence of these terms, a detailed examination for a gun problem shows these terms to have magnitudes comparable to other terms in the equations during at least part of the ignition sequence. The equations compare as follows:

Gas Momentum

$$\rho\phi\frac{Du}{Dt} =$$

$$\text{Krier:} \quad -\frac{\partial}{\partial x}(\phi p) - \mathcal{D} + (u-u_m)\dot{m}_b + \frac{\partial}{\partial x}\left[(u-u_m)^2\rho\phi\right] - \psi u, \tag{1}$$

$$\text{Gough:} \quad -\phi\frac{\partial p}{\partial x} - \mathcal{D} + (u-u_p)\dot{m}_b - \psi u\ . \tag{2}$$

Solid Momentum

$$\rho_p(1-\phi)\frac{Du_p}{Dt} =$$

$$\text{Krier:} \quad -(u_p-u_m)\dot{m}_b + \mathcal{D}\left(\frac{1-\phi}{\phi}\right) + \frac{\partial}{\partial x}\left[(1-\phi)\rho_p(u_p-u_m)^2\right], \tag{3}$$

$$\text{Gough:} \quad -(u-u_p)\dot{m}_b + \mathcal{D} - \frac{\partial}{\partial x}\left[(1-\phi)R\right] - (1-\phi)\frac{\partial p}{\partial x}\ . \tag{4}$$

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9 *Proceedings of Two-Phase Flow and Heat Transfer Symposium-Workshop, October 1976, Ft. Lauderdale, FL, Clean Energy Research Institute, University of Miami, 1976.*

10 *K. K. Kuo, "A Summary of the JANNAF Workshop on Theoretical Modeling and Experimental Measurements of the Combustion and Fluid Flow Processes in Gun Propellant Charges", 13th JANNAF Combustion Meeting, Monterey, CA, September 1976.*

In the gas phase momentum equation the difference is whether the porosity should be inside or outside the pressure gradient. In the debate about the form of the pressure gradient term, it has been noted by Harlow[11] and by Gough[12] that a $P\frac{\partial\phi}{\partial x}$ term would accelerate a system at rest with a non-uniform porosity. Crowe[13] noted that in a weightless environment where such a system can be conceived, there should be no acceleration. In the treatment of drag, adding Krier's momentum equations results in a net drag force on the mixture if his term $\mathcal{D}$ is the same in both equations. Gough's solid phase momentum equation has two additional forces to represent stress from the bed's resistance to compaction and a response to the gas pressure gradient. Having assumed a fluidized bed, Krier omits the stress term.

Similar comparison is not as straight forward for the gas energy equation because Krier uses total energy while Gough uses internal energy as the dependent variable.

$$\text{Krier: } \phi\rho\frac{DE}{Dt} = -\frac{\partial}{\partial x}(up\phi) + \phi\rho(u-u_m)E + (u-u_m)\phi p - \phi\rho(u-u_m^3) + \phi\rho u(u-u_m)^2 - q_{gp} + \dot{m}_b\left(0.9\, e_{chem} - e + \frac{(u-u_p)^2}{2}\right) . \tag{5}$$

Gough's form can be converted to total energy,

$$\phi\rho\frac{DE}{Dt} = -p\frac{D\phi}{Dt} + \frac{\phi\rho}{A}\frac{\partial}{\partial x}(Au) + Du_p - q + \dot{m}_b\left[e_{chem} - e + \frac{p}{\rho} + \left(\frac{u_p^2 - u^2}{2}\right)\right] - \phi\frac{\partial p}{\partial x} . \tag{6}$$

There are several differences an analysis of which would be quite lengthy.

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[11] *F. H. Harlow and A. A. Amsden, "Numerical Calculations of Multiphase Flow", J Comp Phys, 17, (1), January 1973.*

[12] *P. S. Gough, "The Predictive Capability of Models of Interior Ballistics", 12th JANNAF Combustion Meeting, Newport, RI, CPIA Publication 273, December 1975.*

[13] *C. T. Crowe, Washington State University, private communication, 1976.*

No such parallel comparison arises for solid phase energy conservation. Gough (and others[2,4]) treat the solid only as a problem in transient heat conduction before ignition. When the computed surface temperature reaches the specified ignition temperature, combustion takes over and heat is exchanged between the two phases only by the heat release of combustion. Krier uses an equation similar to that of the gas to conserve energy of the particles. Solid phase bulk temperature is the dependent variable that affects heat transfer from the gas and is compared to some criterion for ignition. In a comparison of the surface with bulk temperature ignition criterion, reported earlier[14], a 4K bulk temperature rise was found equivalent to a 155K surface temperature rise in the same time for a gun propelling charge.

The Problem

The laboratory experiment loaded a 25mm diameter chamber 190mm long with seven-perforated M30 propellant. After a 38g tetryl pellet was detonated at one end, pressure-time was measured at four axial stations in the bed (63mm, 100mm, 138mm, 176mm).

Code input values are given in Table I. Inputs for Gough's code were the values reported by Krier except where noted.

RESULTS AND DISCUSSION

Pressure

Figure 1 compares the predictions of pressure-time at two bed locations for Krier's data of Reference 7 with igniter time of 0.5ms.

Comparison of these predicted results with the experimental pressures is difficult because of the ragged data. In six tests, peak pressures ranged from 40 to 300 MPa at the 63mm gage, and 130 to 220 at the 137mm gage. If the high and low at each gage were disregarded, the range could be 120 to 240 MPa and 170 to 205 MPa respectively.

Estimates for the speed of propagation of the pressure wave in the bed vary from 1 to 33mm/μs with deceleration[8]. Although scatter of the data precludes firm estimates, the predicted rates of less than 1mm/μs are clearly too low. The experimental rates were about the same for inert and live propellant beds.

Krier reported that predicted pressure profiles were little changed when an inert propellant was assumed (Fig. 8, Ref. 7) for an igniter time of 0.1ms. Gough's code shows more sensitivity to the difference. The dotted lines in Figure 2 represent inert propellant

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[14] *C. W. Nelson, "Comparison of Predictions of Three Two-Phase Flow Codes", 13th JANNAF Combustion Meeting, Monterey, CA, September 1976.*

Table I. Code Input Data

Propellant		
Outer Diameter	7.01mm	
Perforation Diameter	1.32mm	
Length	15.85mm	
Density	$1.66 g/cm^3$	
Burning Rate Coefficient	$0.70 \frac{cm}{s(MPa)^n}$	Note a
Burning Rate Exponent	0.667	
Weight	99g	
Ignition Temperature	450K	Note b
Speed of Sound when Packed	442m/s	
Settling Porosity	0.42	Note c
Bed Geometry		
Length	200mm	
Initial Temperature	305K	
Initial Porosity	0.47	
Diameter	25mm	
Thermodynamics		
Energy Release in Burning	4736J/g	Note a
Gas Molecular Weight	23.2	
Gas Specific Heat Ratio	1.23	
Igniter Energy	3682J/g	Note d
Covolume	$1.01 cm^3/g$	Note d
Igniter Discharge Rate		
Rate	17.84kg/cm/s	
Length	12.5mm	

Notes:

a. Incorrectly stated in Ref. 7.

b. Gough Surface Criterion 450K.

c. Not used in Krier code.

d. Not stated in Ref. 7.

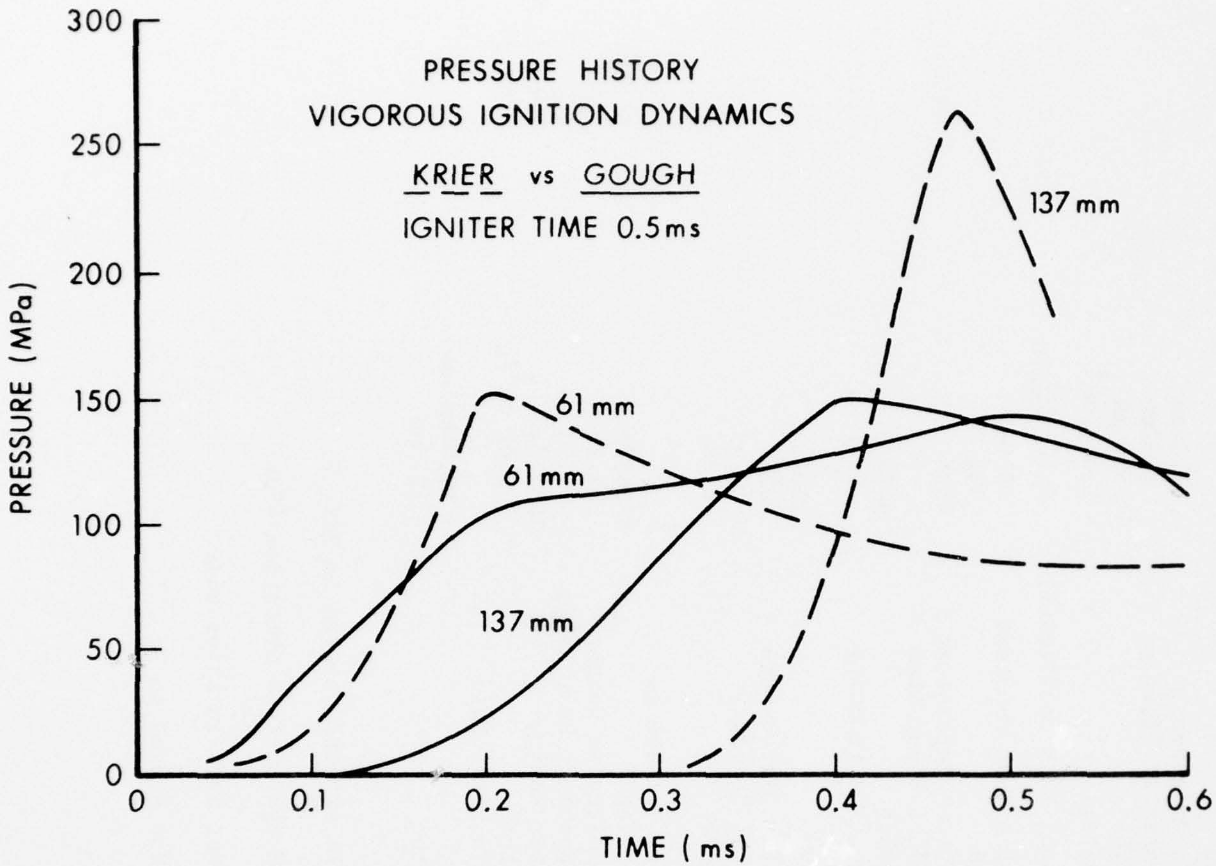

Figure 1. Pressure History Comparisons, Igniter Time 0.5ms

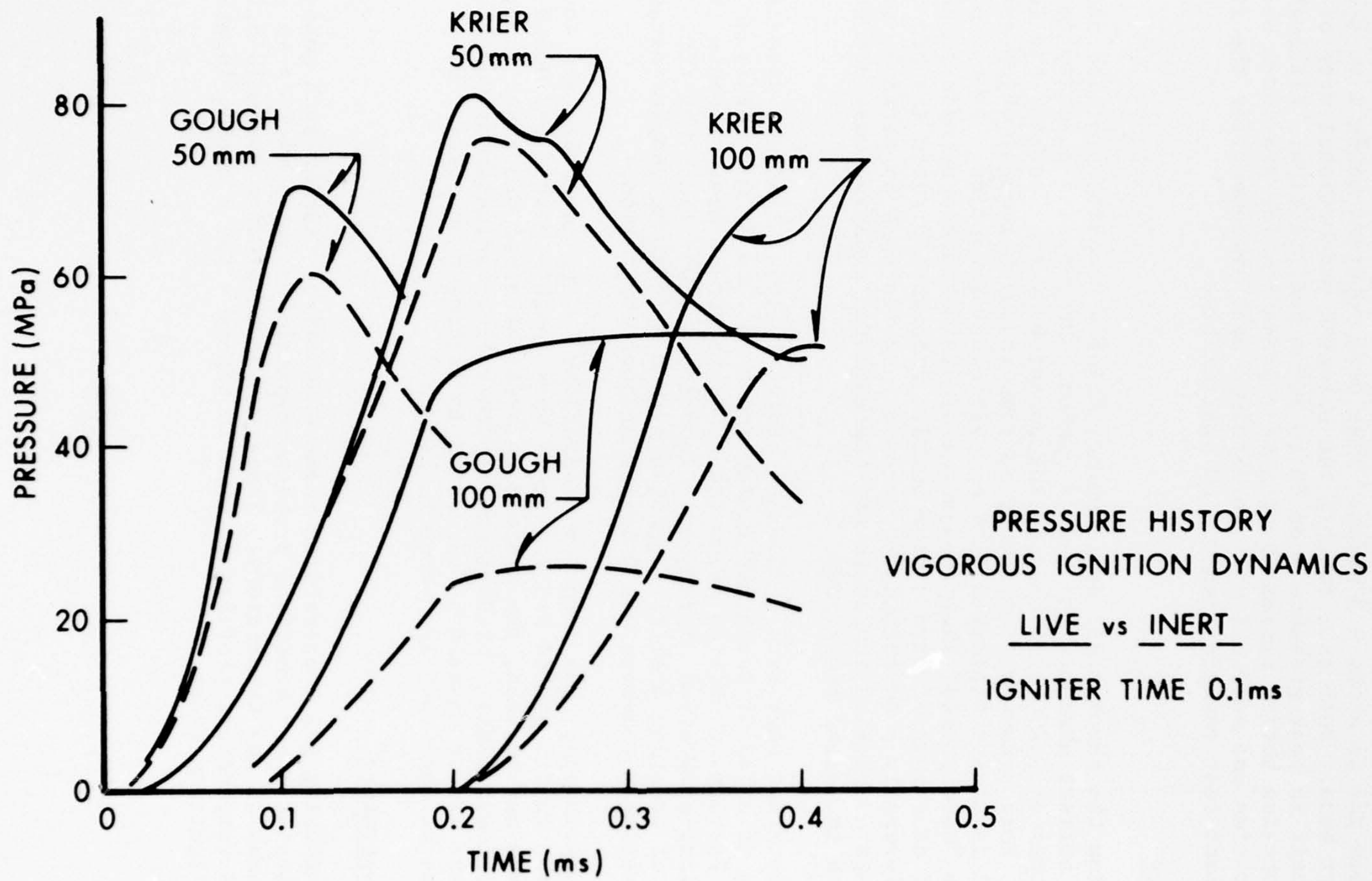

Figure 2. Pressure History Comparisons for Live and Inert Propellant

simulations. Gough's propagation speed for the pressure wave is about 0.6 mm/μs while Krier's is about 0.3 mm/μs. The sound speed in the undisturbed gas is about 0.3 mm/μs. Test data reported rates 1 to 3 mm/μs in inert beds. Both show roughly the observed proportional drop of about half in peak pressure from 50 to 100mm bed position. Although Krier obtains better agreement with test pressures for the inert bed, igniter time was only 0.1 ms. He obtained best agreement for the live propellant test results with 0.5 ms igniter time.

Porosity

From the theoretical development, Krier's porosity profiles should not be correct wherever the bed is packed. He computes porosity in the bed center as 0.250 when the initial porosity of the "packed" bed is 0.470. Such a compression cannot be computed with a model which assumes the bed is always fluidized with no particle interaction. As the bed becomes "more packed" the propagation of disturbances proceeds through the bed as though it were a true solid. Propagation rates are probably inversely proportional to porosity. Resistance to particle motion increases as packing increases and the momentum equation must account for such increased resistance.

The Krier code sets 0.25 as an arbitrary lower limit on porosity. Packing of a bed of these particular grains occurs at a porosity above 0.40. For any porosities below the 0.40, the model misrepresents the mechanical properties of the bed. Imposing a lower limit has the effect of creating arbitrary gradients that affect the coupled equations. It effectively converts solid to gas without combustion.

Surprisingly, the porosity predictions by the two codes are not far apart in the packed bed regions. When Gough's packed bed sound speed was set to zero, the minimum porosity attained was about 0.25, Krier's lower limit. Predictions of other flow variables by Gough's code were little changed by variation in packing properties. Predictions of each code are shown in Figure 3.

Gas Temperature

Computing gas temperatures seems a sensitive task in such numerical calculations. Numerical problems typically show themselves in oscillations in gas temperature. These two codes predict markedly different gas temperature profiles as seen in Figure 4 for a common location of the ignition front.

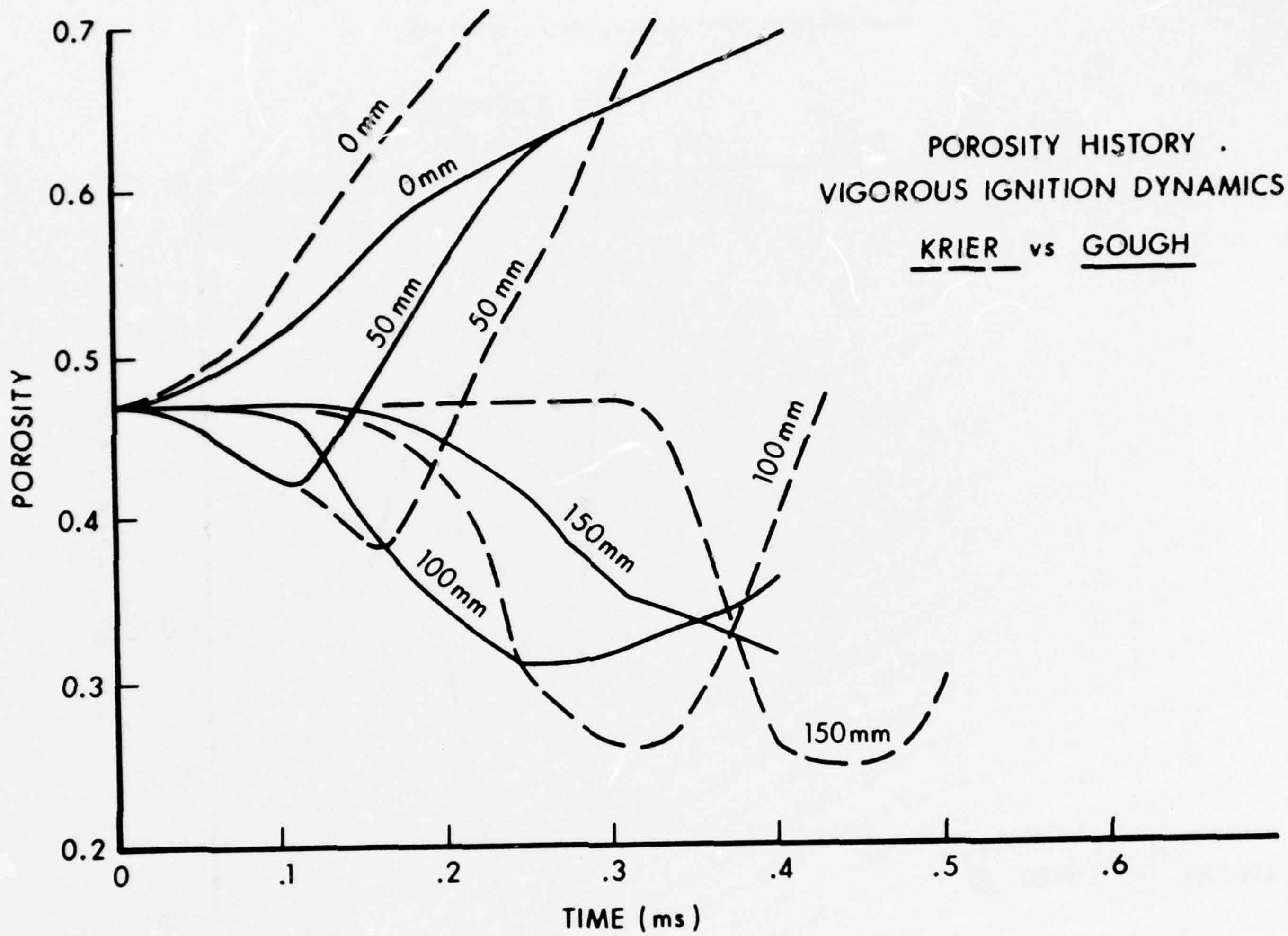

Figure 3. Porosity History Comparisons

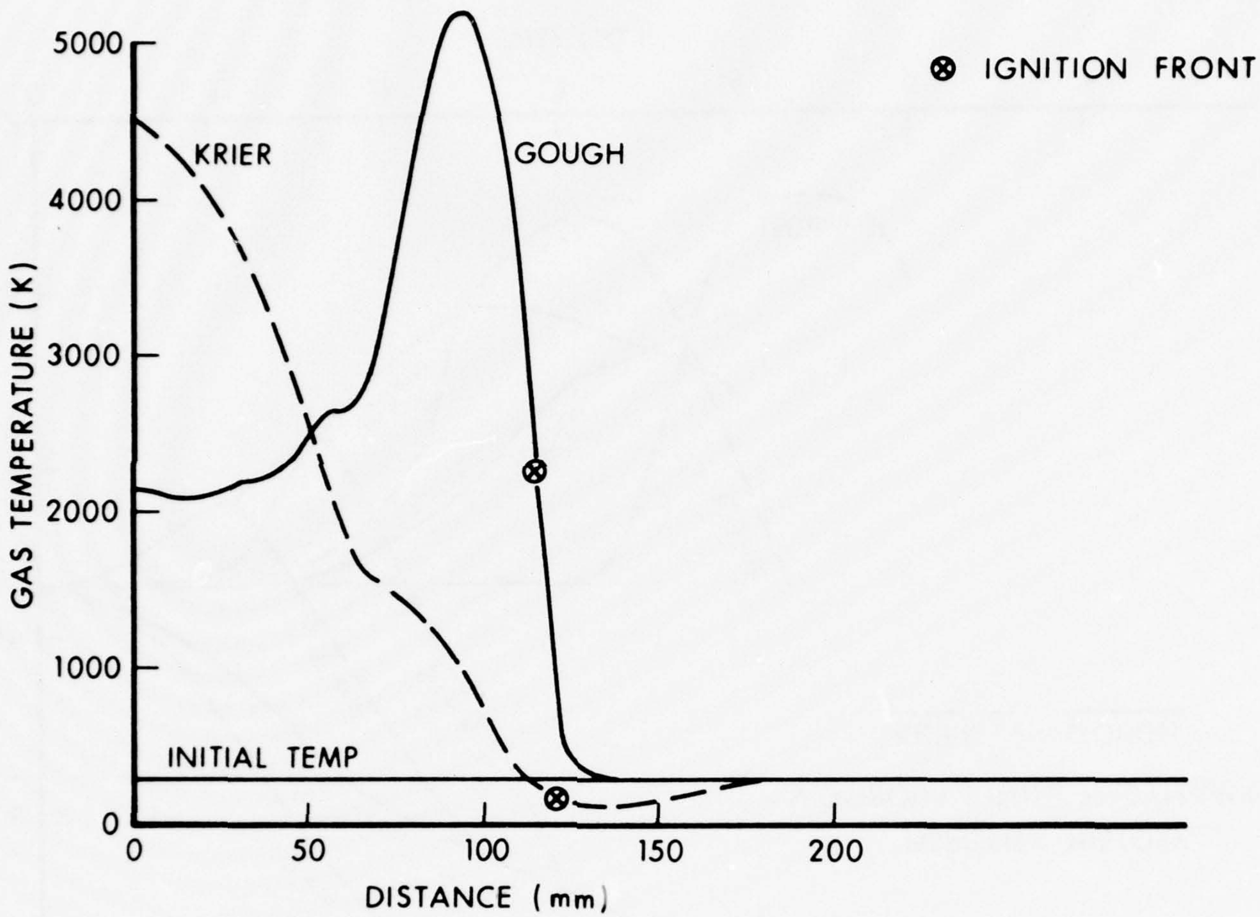

Figure 4. Gas Temperature Comparisons

Krier's temperature profile has two questionable features that need explanation. At the igniter end temperature seems too high. Igniter gas enters at a temperature of about 3400K (E^g_{chem}/c_v). Note that energy, not enthalpy, is the energy added in the equation. With no compressive work on the gas in that region, the temperature should be limited by the temperature of the entering gas. The argument is further supported by later results in the same calculation which predict temperatures over 10000K. A postulation of local compression is contradicted by the monotonic increase of porosity with time. If the region were being compressed, as is the region ahead of the pressurization front, local porosity would decrease.

At the front of the compression wave in the bed interior Krier's predicted gas temperatures and heat transfer violate thermodynamic principles. The initial physical condition is a quiescent gas in thermal equilibrium with solid particles. Hot gas entering at the aft portion forms a compression front driving gas and particles forward. In the forward portion of the bed the gas should be heated by the combination of compression by particle compaction and mixing with the hot combustion gas. As the gas temperatures rise, heat is transferred by convection (only mode allowed) to the particles.

What the code predicts however is a cooling of the gas from 305K to about 140K while the solid phase is being simultaneously heated from 305K to 310K. Heat transfer from a cold gas to a hot particle is inadmissable. Although the printed output in the appendix of Ref. 7 shows only one time step, the full results show the minimum temperature region propagating through the bed but never any particle cooling. Neither the low gas temperature nor the particle heating can be justified by quantitative arguments.

Gough's predictions show a more credible shape of temperature distribution although the magnitude of the peak seems high. There is a compression wave which could locally heat the gas. For a temperature rise, without mass addition, to 1.4 times the uncompressed temperature, the pressure would have to increase by a factor of about ten. Local porosity would have to decrease to much less than the packing porosity to accomplish such a compression. Computed porosity decrease is only a factor of two.

When an excessively large igniter source was assumed (45 and 168 kg/cm/s) the peak temperatures soared to values far in excess of 10000K.

Flame Spreading

Krier reported that flame spreading rate could be correlated with assumed igniter source strength (Fig. 21, Ref. 15). For the mass addition rate used in this comparison, the flame spreading rate of 0.3mm/μs was not sensitive to the igniter time. Gough's code also

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[15] *H. Krier and S. Gokhale, "Vigorous Ignition of Granulated Propellant Beds by Blast Impact", BRL Contract Rpt No. 263, Oct 75, AD #B007026L.*

predicts a dependence of flame spreading rate on igniter strength. For three values used (17.8, 143, and 535 kg/cm/s) the corresponding flame spreading rates are (0.7, 1.1, and 2.4 mm/μs). Figure 5 shows the dependence for both Gough's and Krier's codes. The rate is not dependent on the time duration of the igniter. Figure 6 compares the flame spreading predictions in the bed.

The dominant influence of igniter strength on flame spreading rate can be explained by the relative gas production rates of igniter and propellant. Considering the grain surface, propellant density, and burning rate, combustion gases are produced at a rate of 0.041 $P^{.67}$ kg/cm/sec which at 100 MPa is only 0.9 kg/cm/sec whereas the igniter input is 17.8 kg/cm/sec. As the wave propagates thru the bed the rate of increase of gas in the region behind the wave is controlled by the flow of gas down the pressure gradient. In a cell where the pressure rise rate is 6 MPa/sec (a typical computed rate) the gas increase rate is of the order of 8 kg/cm/sec of which only about 0.9 kg/cm/sec is provided by the combustion. Even these crude estimates show the dominance of the igniter in this range of source strengths.

Phase Velocities

Krier did not publish plots of gas and solid velocities. Figures 7, 8, and 9 show Gough's predicted values at 0.05, 0.11, and 0.18 ms for both velocity fields.

CONCLUSIONS

1. Flow predictions are different for the Gough and Krier codes.

2. Krier's gas temperature predictions in the bed interior are incorrect.

3. Both codes predict a linear dependence of flame spreading rate on igniter strength. Gough's rates are about twice Krier's.

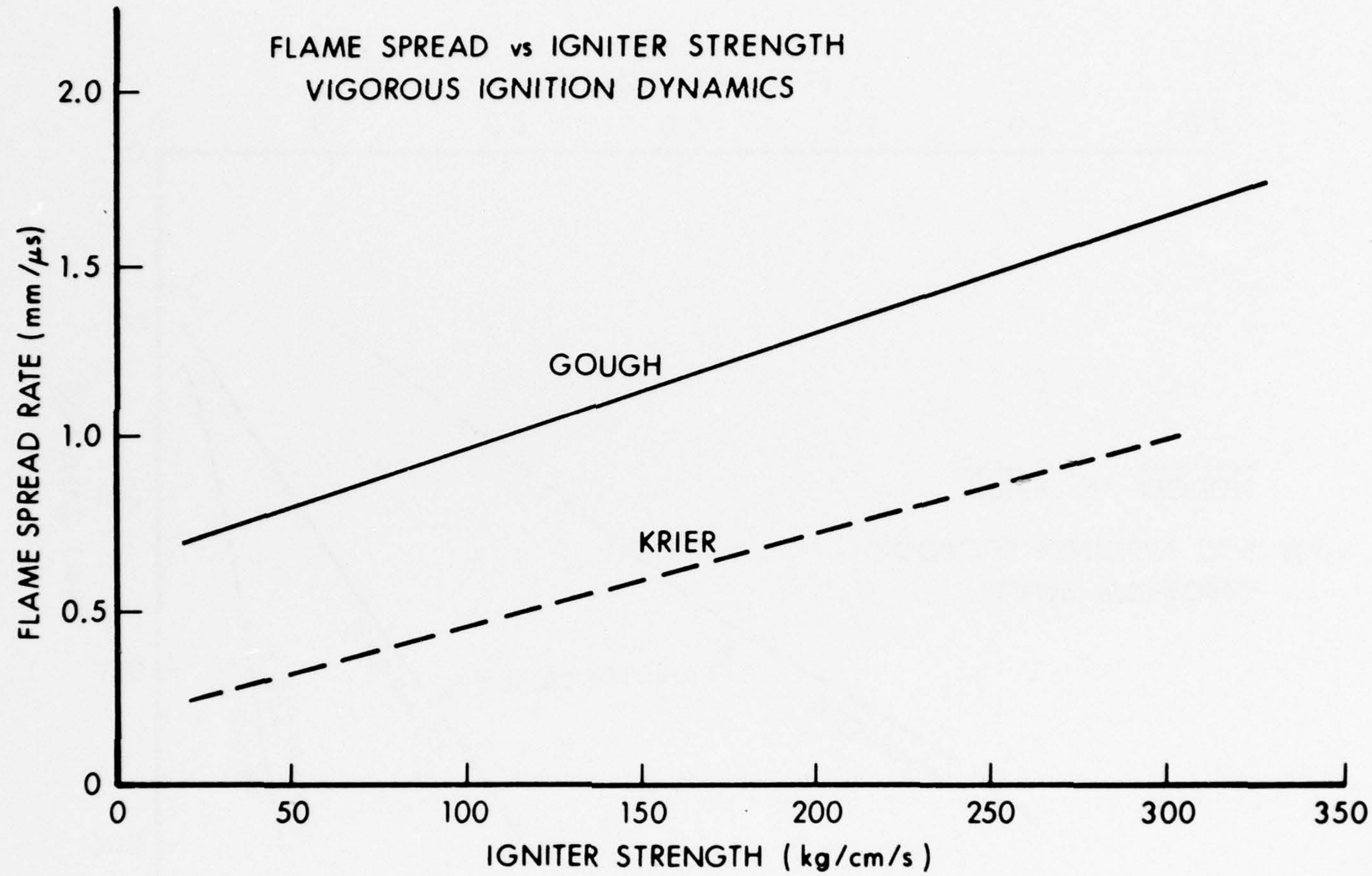

Figure 5. Flame Rate Dependence on Igniter Strength

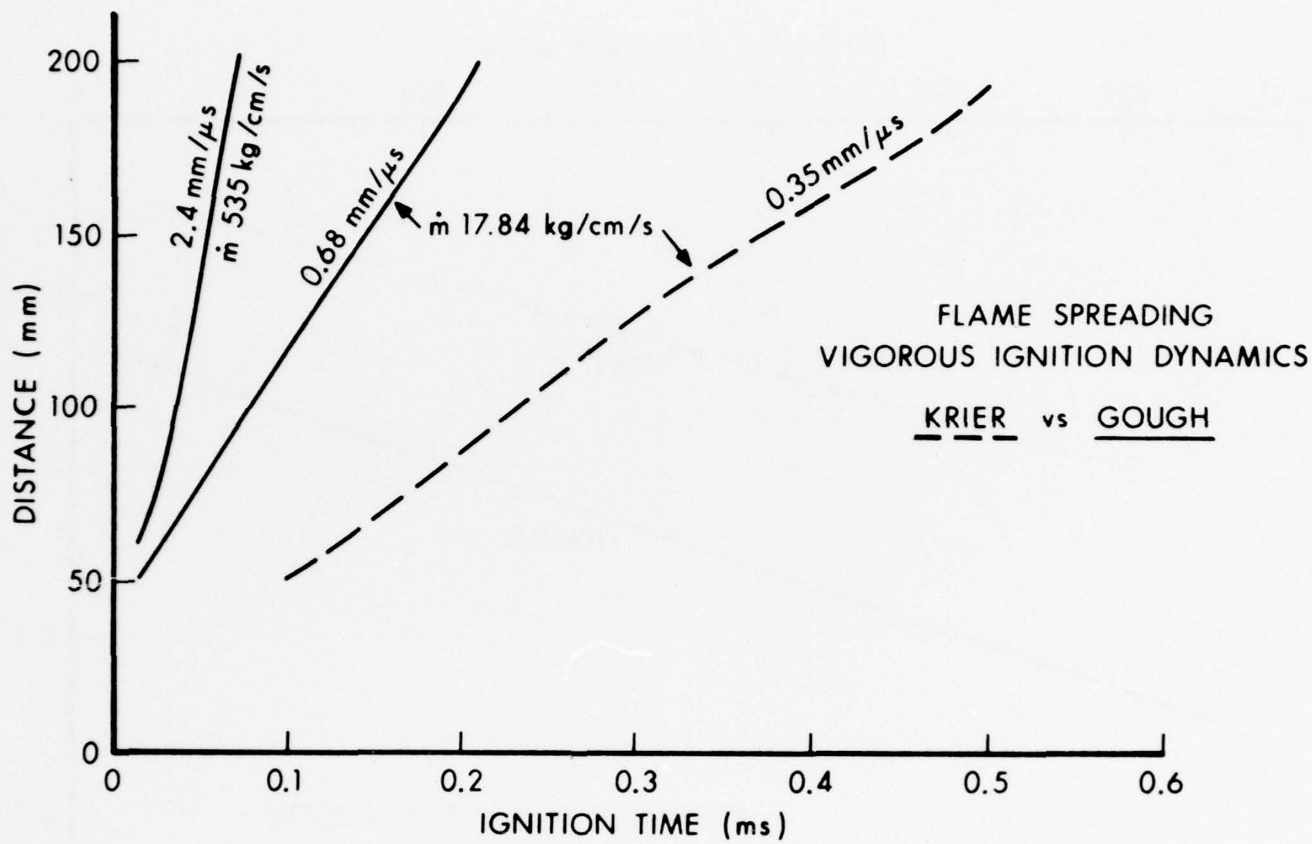

Figure 6. Flamespreading

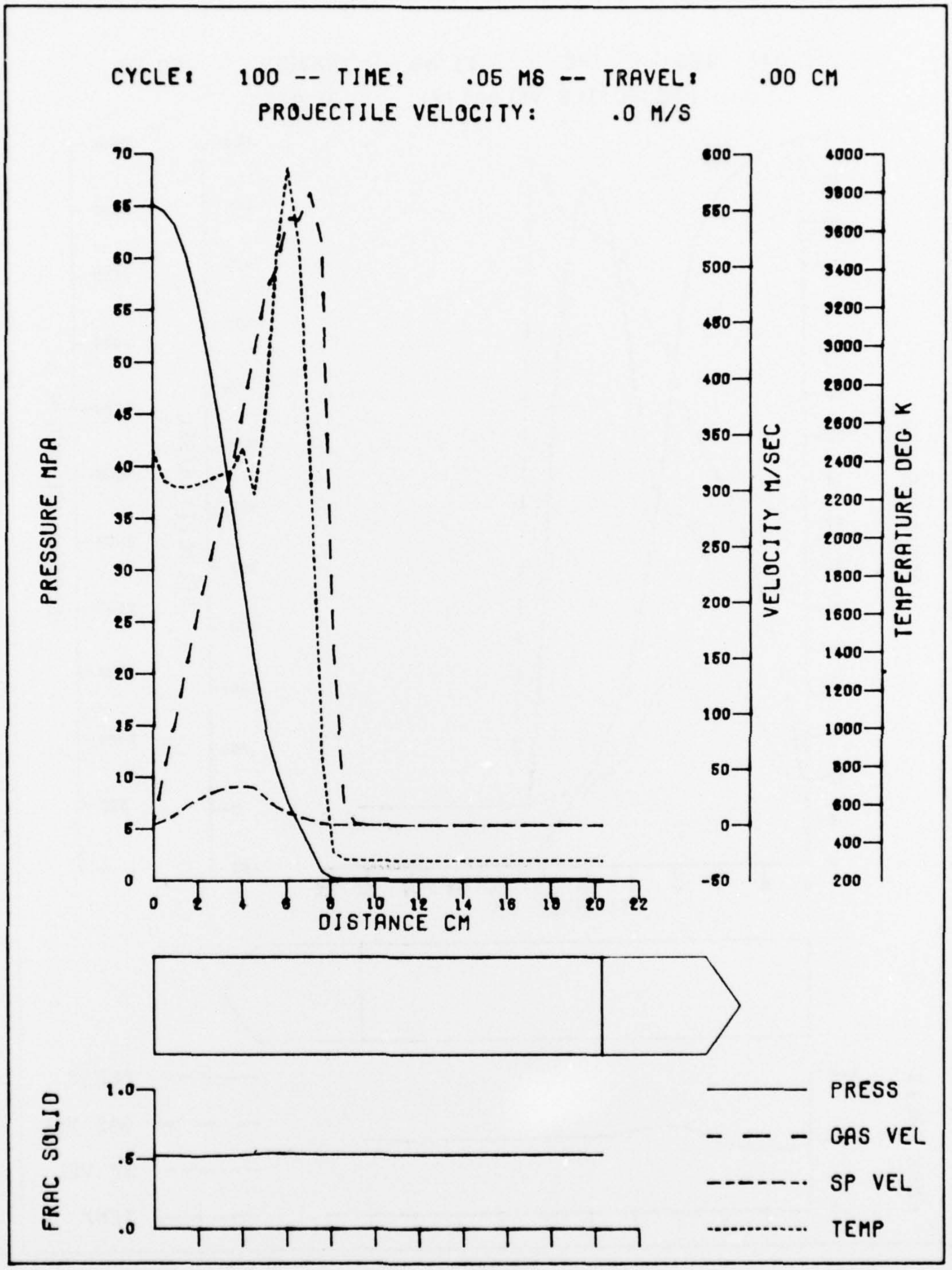

Figure 7. Gough's Flow Field at 0.05ms

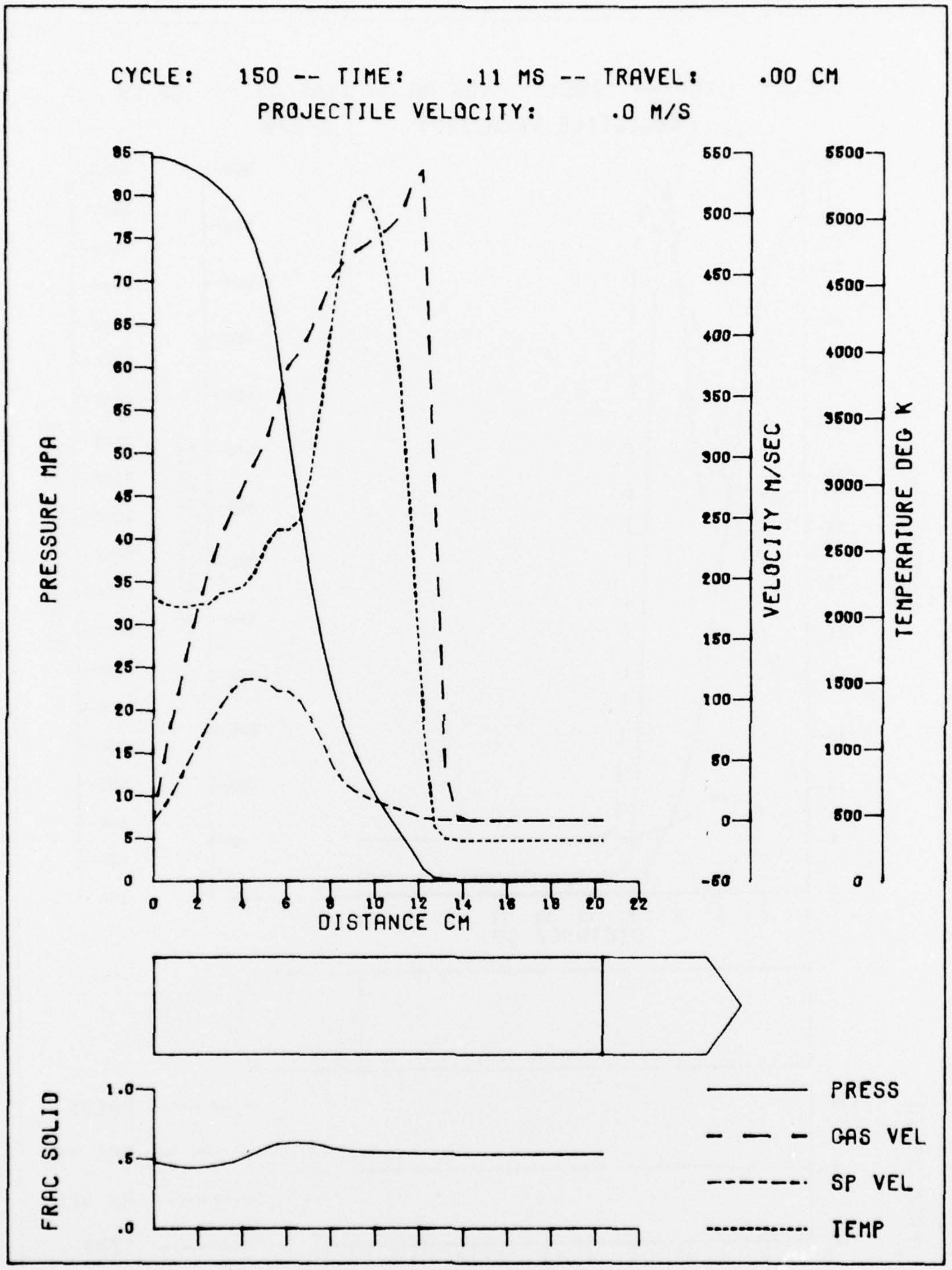

Figure 8. Gough's Flow Field at 0.11ms

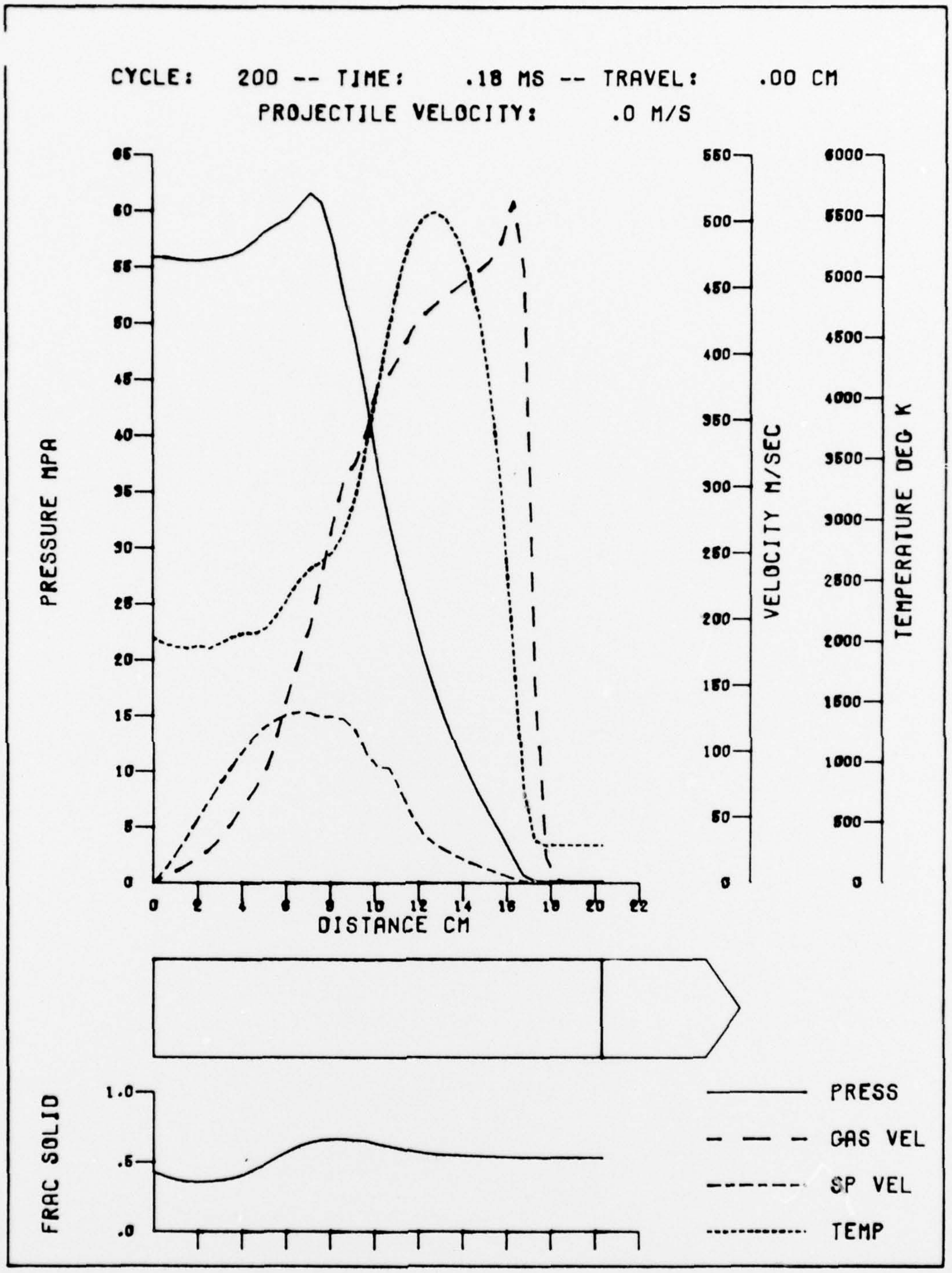

Figure 9. Gough's Flow Field at 0.18ms

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